Towards improved Hashin–Shtrikman bounds on the effective moduli of random composites

Sébastien Brisard

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Aug. 27, 2015

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The curse of isotropy

Séba[…]

Aug. 27, 2015

Navier — Université Paris-Est — École des Ponts ParisTech — IFSTTAR — CNRS dépasser les frontières

Towards improved Hashin–Shtrikman bounds o… ffective m… of ra… es

The cur… isotropy

The story of a failure

Aug. 27, 2015

Navier

UNIVERSITÉ PARIS-EST

École des Ponts ParisTech

IFSTTAR

cnrs

The principle of minimum potential/complementary energy

Requires kinematically/statically admissible trial fields!

The principle of Hashin & Shtrikman (1962)

Effective stiffness

Stiffness of reference material

$$\mathbf{C}_0 \begin{smallmatrix}\leq \\ \geq\end{smallmatrix} \mathbf{C} \quad \Rightarrow \quad \mathcal{H}(\hat{\boldsymbol{\tau}}) \begin{smallmatrix}\leq \\ \geq\end{smallmatrix} \frac{1}{2}\mathbf{E} : \mathbf{C}^{\mathrm{eff}} : \mathbf{E}$$

No requirements on the trial field!

Local stiffness

Trial field (stress polarization)

Functional of H&S (TBD later)

Hashin & Shtrikman (1962), *J. Mech. Phys. Sol.* **10(4)** **Willis (1977),** *J. Mech. Phys. Sol.* **25(3)**

Motivation

Construction of a (microstructure-dependent) trial field

Phase-wise constant trial fields: the most simple trial field

$$\hat{\boldsymbol{\tau}}(\boldsymbol{x}) = \sum_{\alpha=1}^{N} \chi_\alpha(\boldsymbol{x})\,\hat{\boldsymbol{\tau}}_\alpha$$

Indicator function of phase α

Constant (to be optimized)

Local descriptors of the microstructure

The χ_α at the observation point.

Macroscopic descriptors (Hashin and Shtrikman, 1962)

Volume fractions only (isotropic materials)!

Hashin & Shtrikman (1962), *J. Mech. Phys. Sol.* **10(4)** **Willis (1977),** *J. Mech. Phys. Sol.* **25(3)**

Phase-wise constant trial fields

- do not depend on neighborhood
- no (relative) length-scale in the resulting bounds

Additional local descriptors

- should remain simple (for evaluation of $\mathcal{H}(\hat{\boldsymbol{\tau}})$)
- aggregate microstructural info at and around observation point

The most simple such local descriptor

- local volume fraction
- arguably physically meaningful (Widjajakusuma et al., 1999)

Widjajakusuma et al. (1999), *Comput. Mater. Sci.* **16(1-4)**

Motivation
Local volume fraction

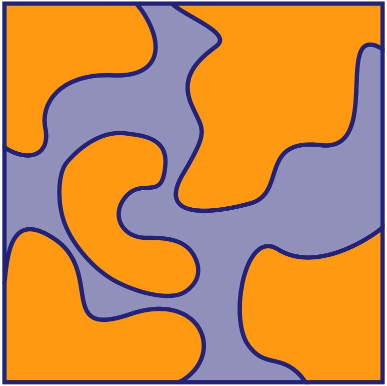
Spherical windows

Radius of spherical window

Indicator function of phase α

$$\tilde{f}_\alpha(x, a) = \frac{1}{W} \int_{\|r\| \leq a} \chi_\alpha(x + r) \, \mathrm{d}V_r$$

Volume of spherical window



The case of two-phase materials

$$\tilde{f}(x, a) = \tilde{f}_1(x, a) = 1 - \tilde{f}_2(x, a)$$

Spherical windows

Radius of spherical window

Indicator function of phase α

$$\tilde{f}_\alpha(x, a) = \frac{1}{W} \int_{\|r\| \leq a} \chi_\alpha(x + r) \, \mathrm{d}V_r$$

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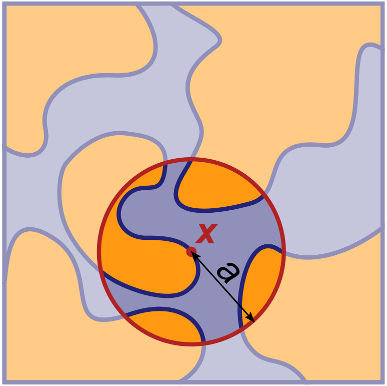

The case of two-phase materials

$$\tilde{f}(x, a) = \tilde{f}_1(x, a) = 1 - \tilde{f}_2(x, a)$$

Roadmap to improved bounds

Step 1 – Defining enriched trial fields

Step 2 – Evaluating the H&S functional $\rightarrow$ The curse of isotropy!

Step 3 – Optimizing the resulting bound

Step 1 – Defining enriched trial fields

Original trial field

$$\hat{\boldsymbol{\tau}}(\boldsymbol{x}) = \sum_{\alpha=1}^{2} \chi_\alpha(\boldsymbol{x})\hat{\boldsymbol{\tau}}_\alpha$$

Enriched trial field

Constant (to be optimized)

$$\hat{\boldsymbol{\tau}}(\boldsymbol{x}) = \sum_{\alpha=1}^{2} \sum_{h=1}^{p} \chi_\alpha(\boldsymbol{x})\tilde{f}(\boldsymbol{x}, a)^h \hat{\boldsymbol{\tau}}_{\alpha h}$$

The functional of Hashin & Shtrikman

$$\mathcal{H}(\hat{\boldsymbol{\tau}}) = \frac{1}{2}\boldsymbol{E} : \mathbb{C}_0 : \boldsymbol{E} + \boxed{\boldsymbol{E} : \overline{\hat{\boldsymbol{\tau}}}} - \frac{1}{2}\boxed{\overline{\hat{\boldsymbol{\tau}} : (\mathbb{C} - \mathbb{C}_0)^{-1} : \hat{\boldsymbol{\tau}}}} - \frac{1}{2}\boxed{\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]}}$$

The functional of Hashin & Shtrikman

$$\sum_{\alpha,h,k} Y_{\alpha,h+k}\hat{\boldsymbol{\tau}}_{\alpha h} : (C_\alpha - C_0)^{-1} : \hat{\boldsymbol{\tau}}_{\alpha k}$$

$$\sum_{\alpha,h} Y_{\alpha h}\boldsymbol{E} : \hat{\boldsymbol{\tau}}_{\alpha h}$$

$$\mathcal{H}(\hat{\boldsymbol{\tau}}) = \frac{1}{2}\boldsymbol{E} : C_0 : \boldsymbol{E} + \boxed{\boldsymbol{E} : \overline{\hat{\boldsymbol{\tau}}}} - \frac{1}{2}\boxed{\overline{\hat{\boldsymbol{\tau}} : (C - C_0)^{-1} : \hat{\boldsymbol{\tau}}}} - \frac{1}{2}\boxed{\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]}}$$

One-point descriptors of the microstructure

$$Y_{\alpha h} = \langle \chi_\alpha(x)\tilde{f}(x, a)^h \rangle$$

Step 2 – Evaluating the H&S functional

The trivial terms

The functional of Hashin & Shtrikman

$$\sum_{\alpha,h,k} Y_{\alpha,h+k} \hat{\boldsymbol{\tau}}_{\alpha h} : (C_\alpha - C_0)^{-1} : \hat{\boldsymbol{\tau}}_{\alpha k}$$

$$\sum_{\alpha,h} Y_{\alpha h} \boldsymbol{E} : \hat{\boldsymbol{\tau}}_{\alpha h}$$

$$\mathcal{H}(\hat{\boldsymbol{\tau}}) = \frac{1}{2}\boldsymbol{E} : C_0 : \boldsymbol{E} + \boxed{\boldsymbol{E} : \overline{\hat{\boldsymbol{\tau}}}} - \frac{1}{2}\boxed{\overline{\hat{\boldsymbol{\tau}} : (C - C_0)^{-1} : \hat{\boldsymbol{\tau}}}} - \frac{1}{2}\boxed{\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]}}$$

???

One-point descriptors of the microstructure

$$Y_{\alpha h} = \langle \chi_\alpha(x) \tilde{f}(x, a)^h \rangle$$

Step 2 – Evaluating the H&S functional

The not-so-trivial term

The Green operator for strains as a “convolution” operator

$$\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \frac{1}{V} \int_{x,y \in \Omega} \hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x, y) : \hat{\boldsymbol{\tau}}(y) \, \mathrm{d}V_x \, \mathrm{d}V_y$$

Step 2 – Evaluating the H&S functional

The not-so-trivial term

The Green operator for strains as a “convolution” operator

$$\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \frac{1}{V} \int_{x,y \in \Omega} \hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x, y) : \hat{\boldsymbol{\tau}}(y) \, \mathrm{d}V_x \, \mathrm{d}V_y$$

If Ω is indeed a RVE, then $\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \langle \overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} \rangle$

$$\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \frac{1}{V} \int_{x,y \in \Omega} \langle \hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x, y) : \hat{\boldsymbol{\tau}}(y) \rangle \, \mathrm{d}V_x \, \mathrm{d}V_y$$

Step 2 – Evaluating the H&S functional

The not-so-trivial term

The Green operator for strains as a “convolution” operator

$$\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \frac{1}{V}\int_{x,y\in\Omega} \hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x,y) : \hat{\boldsymbol{\tau}}(y)\,\mathrm{d}V_x\,\mathrm{d}V_y$$

If Ω is indeed a RVE, then $\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \langle\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]}\rangle$

$$\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \frac{1}{V}\int_{x,y\in\Omega} \langle\hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x,y) : \hat{\boldsymbol{\tau}}(y)\rangle\,\mathrm{d}V_x\,\mathrm{d}V_y$$

$$\langle\hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x,y) : \hat{\boldsymbol{\tau}}(y)\rangle = \sum_{\alpha,\beta,h,k} Z_{\alpha h,\beta k}(x-y)\hat{\boldsymbol{\tau}}_{\alpha h} : \boldsymbol{\Gamma}_0(x,y) : \hat{\boldsymbol{\tau}}_{\beta k}$$

Two-point descriptors of the microstructure

$$Z_{\alpha h,\beta k}(r) = \langle\chi_\alpha(x)\tilde{f}(x,a)^h\chi_\beta(x+r)\tilde{f}(x+r,a)^k\rangle$$

For isotropic microstructures

$$Z_{\alpha h,\beta k}(\boldsymbol{r}) = Z_{\alpha h,\beta k}(\|\boldsymbol{r}\|)$$

Two-point descriptors vanish!

Hill tensor of spheres

$$\frac{1}{V}\int Z_{\alpha h,\beta k}(x-y)\Gamma_0(x,y)\,\mathrm{d}V_x\,\mathrm{d}V_y = \left(Y_{\alpha,h+k}\delta_{\alpha\beta} - Y_{\alpha h}Y_{\beta k}\right)\boldsymbol{P}_0$$

Step 2 – Evaluating the H&S functional

Putting it all together

$$\sum_{\alpha,h,k} Y_{\alpha,h+k}\hat{\boldsymbol{\tau}}_{\alpha h} : (C_\alpha - C_0)^{-1} : \hat{\boldsymbol{\tau}}_{\alpha k}$$

$$\sum_{\alpha,h} Y_{\alpha h} \boldsymbol{E} : \hat{\boldsymbol{\tau}}_{\alpha h}$$

$$\mathcal{H}(\hat{\boldsymbol{\tau}}) = \frac{1}{2}\boldsymbol{E} : C_0 : \boldsymbol{E} + \boxed{\boldsymbol{E} : \overline{\hat{\boldsymbol{\tau}}}} - \frac{1}{2}\boxed{\overline{\hat{\boldsymbol{\tau}} : (C - C_0)^{-1} : \hat{\boldsymbol{\tau}}}} - \frac{1}{2}\boxed{\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]}}$$

$$\sum_{\alpha,h,\beta,k} \left(Y_{\alpha,h+k}\delta_{\alpha\beta} - Y_{\alpha h}Y_{\beta k}\right)\hat{\boldsymbol{\tau}}_{\alpha h} : P_0 : \hat{\boldsymbol{\tau}}_{\beta k}$$

Step 3 – Optimizing the bound w.r.t $\hat{\boldsymbol{\tau}}_{\alpha h}$

Stationarity conditions

$$\sum_k Y_{\alpha,h+k}\left(\left(C_\alpha - C_0\right)^{-1} + P_0\right) : \hat{\boldsymbol{\tau}}_{\alpha k} = Y_{\alpha h}\left(E + \sum_{\beta,k} Y_{\beta k} P_0 : \hat{\boldsymbol{\tau}}_{\beta k}\right)$$

Solving the linear system

$\hat{\boldsymbol{\tau}}_{\alpha k} = \mathbf{0}$ for $k \neq 0$!

Remember

$$\hat{\boldsymbol{\tau}}(x) = \sum_{\alpha,k} \chi_\alpha(x)\tilde{f}(x,a)^k \hat{\boldsymbol{\tau}}_{\alpha k}$$

Standard bounds of H&S are retrieved :-(

Conclusion and perspectives

All these developments for nothing?

- Enrichment led to no improvement!
- Extends to a wider class of trial fields!

However…

- Approach might apply to other situations.
- Was well worth trying (if only to spare the time of others!).

Perspectives

- Analysis suggests enrichments with better prospects (maybe).
- Isotropy is the root of our misfortunes: anisotropic descriptors?

$$\langle \chi_\alpha(\boldsymbol{x}) \Phi_h(\boldsymbol{x}) \chi_\beta(\boldsymbol{x} + r\boldsymbol{n}) \Phi_k(\boldsymbol{x} + r\boldsymbol{n}) \rangle = \text{func.}(r, \boldsymbol{n})$$

Thank you for your attention!

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Paper number 68474 (also on HAL)

Appendix

The local problem on the RVE (with shorthand notations)

Field equations

$$
\begin{aligned}
\nabla \cdot \boldsymbol{\sigma}(x) &= \mathbf{0} \\
\boldsymbol{\sigma}(x) &= \mathbf{C}(x) : \boldsymbol{\varepsilon}(x) \iff \nabla \cdot (\mathbf{C} : \nabla^{\mathrm{s}} \boldsymbol{u}) = \mathbf{0} \\
\boldsymbol{\varepsilon}(x) &= \nabla^{\mathrm{s}} \boldsymbol{u}(x)
\end{aligned}
$$

Boundary conditions

$$
\boldsymbol{u}(x) = \boldsymbol{E} \cdot x \iff \boldsymbol{u} \text{ k.a. with } \boldsymbol{E}
$$

k.a. = *kinematically admissible*.

Effective properties

$$
\mathbf{C}^{\mathrm{eff}} = \overline{\boldsymbol{\sigma}} = \overline{\mathbf{C} : \boldsymbol{\varepsilon}}
$$

Introducing an arbitrary, homogeneous reference material C_0.

The Green operator for strains

$$\left.\begin{array}{c}\nabla\cdot(C_0:\nabla^{\mathrm{s}}\boldsymbol{u}+\boldsymbol{\tau})\\ \boldsymbol{u}\text{ k.a. with }\mathbf{0}\end{array}\right\}\iff\boldsymbol{\varepsilon}=-\Gamma_0[\boldsymbol{\tau}]$$

The Lippmann–Schwinger equation

$$\left.\begin{array}{c}\nabla\cdot(C:\nabla^{\mathrm{s}}\boldsymbol{u})\\ \boldsymbol{u}\text{ k.a. with }\boldsymbol{E}\end{array}\right\}\iff\boldsymbol{\varepsilon}=\boldsymbol{E}-\Gamma_0[(C-C_0):\boldsymbol{\varepsilon}]$$

$$\iff\left\{\begin{array}{c}(C-C_0)^{-1}:\boldsymbol{\tau}+\Gamma_0[\boldsymbol{\tau}]=\boldsymbol{E}\\ \boldsymbol{\tau}=(C-C_0):\boldsymbol{\varepsilon}\end{array}\right.$$

Appendix

Local volume fraction is a random variable

Basic properties

$$\langle \tilde{f}_\alpha(x, a) \rangle = f_\alpha$$
$$\langle \tilde{f}_\alpha^2(x, 0) \rangle = f_\alpha$$
$$\langle \tilde{f}_\alpha^2(x, +\infty) \rangle = 0$$

Example: hard spheres

- d: diameter,
- $f = 0.4$,
- 2048 spheres,
- 10000 realizations.